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Contract N00014-86-K-0043

TECHNICAL REPORT No. 101

Electron Energy Levels in a Quantum Well Within an In-Plane Magnetic Field

by

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Prepared for Publication

in

Journal of Applied Physics

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State University of New York at Buffalo
Buffalo, New York 14260

June 1989

UNCLASSIFIED
SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1a. REPORT SECURITY CLASSIFICATION Unclassified	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION / AVAILABILITY OF REPORT Approved for public release; distribution unlimited
2b. DECLASSIFICATION / DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S) UBUFFALO/DC/89/TR-101	5. MONITORING ORGANIZATION REPORT NUMBER(S)
6a. NAME OF PERFORMING ORGANIZATION Depts. Chemistry & Physics State University of New York 6b. OFFICE SYMBOL (*If applicable*)	7a. NAME OF MONITORING ORGANIZATION
6c. ADDRESS (*City, State, and ZIP Code*) Fronczak Hall, Amherst Campus Buffalo, New York 14260	7b. ADDRESS (*City, State, and ZIP Code*) Chemistry Program 800 N. Quincy Street Arlington, Virginia 22217
8a. NAME OF FUNDING / SPONSORING ORGANIZATION Office of Naval Research 8b. OFFICE SYMBOL (*If applicable*)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER Contract N00014-86-K-0043
8c. ADDRESS (*City, State, and ZIP Code*) Chemistry Program 800 N. Quincy Street Arlington, Virginia 22217	10. SOURCE OF FUNDING NUMBERS PROGRAM ELEMENT NO. / PROJECT NO. / TASK NO. / WORK UNIT ACCESSION NO.

11. TITLE (*Include Security Classification*)
Electron Energy Levels in a Quantum Well Within an In-Plane Magnetic Field

12. PERSONAL AUTHOR(S)
H. R. Lee, H. G. Oh, Thomas F. George and C. I. Um

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (*Year, Month, Day*)	15. PAGE COUNT
	FROM _____ TO _____	June 1989	17

16. SUPPLEMENTARY NOTATION
Prepared for publication in Journal of Applied Physics

17. COSATI CODES		
FIELD	GROUP	SUB-GROUP

18. SUBJECT TERMS (*Continue on reverse if necessary and identify by block number*)
ELECTRON ENERGY LEVELS
QUANTUM WELL
IN-PLANE MAGNETIC FIELD
CYCLOTRON ORBITS
QUANTUM CALCULATION,
BULK LANDAU LEVELS, (KP)

19. ABSTRACT (*Continue on reverse if necessary and identify by block number*)

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20. DISTRIBUTION / AVAILABILITY OF ABSTRACT ☒ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS	21. ABSTRACT SECURITY CLASSIFICATION Unclassified
22a. NAME OF RESPONSIBLE INDIVIDUAL Dr. David L. Nelson	22b. TELEPHONE (*Include Area Code*) (202) 696-4410 22c. OFFICE SYMBOL

DD Form 1473, JUN 86 *Previous editions are obsolete.*

SECURITY CLASSIFICATION OF THIS PAGE
UNCLASSIFIED

Journal of Applied Physics, in press

Electron Energy Levels in a Quantum Well Within an In-Plane Magnetic Field

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Abstract

The exact eigenenergy spectrum of an electron is calculated in a quantum well within an in-plane magnetic field. The numerical solutions for the excited energy states as well as the ground state energy are found for various quantum-well widths and barrier heights. The cyclotron orbits are considerably affected by the quantum well. The energy levels higher than the potential height of the quantum well and the energy levels lower than the potential height of the quantum well show quite different behaviors. These are explained with the properties of the combined potential and the wave function inherent to the system.

PACS Nos.: 73.60.-n, 73.20.Dx, 71.50.+t

I. Introduction

The properties of electrons confined in semiconductor heterostructures have been studied for different situations. The carriers in two-dimensional systems subjected to a magnetic field perpendicular to the layers are completely quantized into Landau levels, which have been extensively studied with respect to the quantized Hall effect[1] and Shubnikov-de-Haas oscillations [2]. In this case, since the magnetic field is in the same direction as the confining electric field, the Hamiltonian can be separated into an electric part leading to subbands and a magnetic part leading to Landau levels. For any other orientation, this separation is not possible any more. Thus, in an external magnetic field parallel to the interface, the situation becomes more complicated. By studying the effects of magnetic field on the optical transitions, we may obtain the details of the subband structure[3,4]. Although an in-plane magnetic field usually has little effect on two-dimensional properties, it can strongly affect the spectrum of intersubband optical transitions[5]. If the magnetic length $a_H = (\hbar/\mu\omega)^{1/2}$, where μ and ω are the effective mass and the cyclotron frequency of an electron, respectively, is made comparable to the quantum well width by increasing the magnitude of the magnetic field, the problem is even more complicated because the confining electric field and the magnetic field contribute almost the same weight to the energy levels of electrons. There are several papers in theory[6-9] as well as in experiment[10-12] which study the effect of in-plane magnetic fields on two-dimensional systems. Recently Klama[8] has reported the quantization rules and analytic expressions of the electron energy spectrum in a thin film within a

longitudinal magnetic field. In his paper, the electronic motion is always inside the quantum well because the potential height is taken to be infinite. The eigenenergies of two-dimensional electrons subjected to a tilted magnetic field are solved analytically in a parabolic potential well[10], which is useful for the analysis of transport measurements in their experiments. Oliveira et al[9] have found the electron binding energy in a quantum well of n-type GaAs-$Al_xGa_{1-x}As$ heterostructures by a self-consistent solution of the Poisson and Schrödinger equations. Most of their calculations were done for a couple of the lowest subbands in various systems.

Since the harmonic oscillator is one of the exactly solvable problems[13], the exact eigenvalues for a quantum well under an in-plane magnetic field can be obtained numerically. In this paper we present the numerical solutions for the energy spectrum of electrons in a quantum well with a finite potential height V_0 and well width W comparable to the magnetic length. The eigenenergy spectrum of an infinite potential well is also calculated for comparison. In the calculations, the normalized potential height ($V_0/\hbar\omega$) and well width ($\sqrt{2}W/a_H$) are used to see the results for an arbitrary potential height V_0 and well width W.

II. Theory

Let us consider a quantum well with well width W and the potential height V_0 in an external applied longitudinal DC magnetic field. The uniform external magnetic field $\vec{B} = (0, 0, B_0)$ oriented in the plane of the layer can be described by the vector potential $\vec{A} = (0, B_0x, 0)$. In the direction parallel to $\vec{B}$ the electrons have a free motion, whereas in the

plane perpendicular to $\vec{B}$ they are subjected to the combined potential of the magnetic field and the quantum well. Then, the Hamiltonian for an electron in a potential well with a magnetic field in the xz-plane can be written as

$$H = \frac{1}{2\mu}(P_x^2 + P_z^2) + \frac{1}{2\mu}\left[P_y + eB_0x\right]^2 + V(x) \tag{1}$$

where μ is the effective mass and V(x) is the potential energy of the electron in the well. Correspondingly, the Schrödinger equation is given by

$$H\psi(\vec{r}) = E\psi(\vec{r}) \quad . \tag{2}$$

Due to the translational symmetry in the y- and z-directions, the wave function can be written as

$$\psi(\vec{r}) = \chi(x)\, e^{i(q_y y + q_z z)} \quad . \tag{3}$$

Substituting this wave function into the Schrödinger equation (2), we obtain the effective one-dimensional Schrödinger equation

$$\frac{d^2\chi(x)}{dx^2} + \frac{2\mu}{\hbar^2}\left[\epsilon - \frac{\mu\omega^2}{2}(x - x_0)^2 + V(x)\right]\chi(x) = 0 \quad , \tag{4}$$

where

$$\epsilon = E - \frac{P_z^2}{2\mu} \quad , \tag{5}$$

and we have used $\omega = eB_0/\mu$ for the cyclotron frequency, $x_0 = a_H^2 q_y$ for the position of the orbit center and $a_H = (\hbar/\mu\omega)^{1/2}$ for the magnetic length. Now the two boundaries caused by the quantum well can be determined depending on the location of the orbit center x_0. For the general case, we assume the left and right boundaries of the well are located at $x_L = a$ and $x_R = b$ $(a<b)$, respectively, i.e.,

$$V(x) = \begin{cases} 0 & \text{for} \quad a < x < b \\ V_0 & \text{for} \quad x < a, \quad b < x \end{cases} \tag{6}$$

Introducing the dimensionless length scale $\xi = \sqrt{2}x/a_H$ for the x-coordinate, the Schrödinger equation for the combined potential is divided into three regions:

$$\frac{d^2\chi_I(\xi)}{d\xi^2} + \left[\frac{\epsilon}{\hbar\omega} - \frac{1}{4}(\xi - \xi_0)^2 \right] \chi_I(\xi) = 0 \quad \text{for} \quad \frac{\sqrt{2}a}{a_H} < \xi < \frac{\sqrt{2}b}{a_H} \tag{7a}$$

$$\frac{d^2\chi_{II}(\xi)}{d\xi^2} + \left[\frac{\epsilon - V_0}{\hbar\omega} - \frac{1}{4}(\xi - \xi_0)^2 \right] \chi_{II}(\xi) = 0 \quad \text{for} \quad \xi < \frac{\sqrt{2}a}{a_H} \tag{7b}$$

$$\frac{d^2\chi_{III}(\xi)}{d\xi^2} + \left[\frac{\epsilon - V_0}{\hbar\omega} - \frac{1}{4}(\xi - \xi_0)^2 \right] \chi_{III}(\xi) = 0 \quad \text{for} \quad \frac{\sqrt{2}b}{a_H} < \xi \quad . \tag{7c}$$

Comparing the above Schrödinger equations (7a), (7b), and (7c) with the Weber equation [14],

$$\frac{d^2\psi(z)}{dz^2} + \left(m + \frac{1}{2} - \frac{1}{4}z^2\right)\psi(z) = 0 \quad , \tag{8}$$

we can identify the eigenvalues of the system:

$$\frac{\epsilon}{\hbar\omega} = m + \frac{1}{2} \qquad \text{for} \quad \frac{\sqrt{2}a}{a_H} < \xi < \frac{\sqrt{2}b}{a_H} \tag{9}$$

and

$$\frac{\epsilon - V_0}{\hbar\omega} = m' + \frac{1}{2} \qquad \text{for} \quad \xi < \frac{\sqrt{2}a}{a_H}, \text{ or } \frac{\sqrt{2}b}{a_H} < \xi \quad . \tag{10}$$

The quantum numbers m and m′ are related each other by,

$$(m - m')\hbar\omega = V_0 \quad . \tag{11}$$

The solution of equation (8) is the well-known Weber function[14]:

$$D_m(z) = 2^{m/2}e^{-z^2/4}\left(\frac{\sqrt{\pi}}{\Gamma(1/2-m/2)}F\left(-\frac{1}{2}m\middle|\frac{1}{2}\middle|\frac{1}{2}z^2\right) - \frac{\sqrt{2\pi}\,z}{\Gamma(-m/2)}F\left(\frac{1}{2} - \frac{1}{2}m\middle|\frac{3}{2}\middle|\frac{1}{2}z^2\right)\right) \tag{12}$$

where $F(a|b|x)$ is the confluent hypergeometric function[15] and $\Gamma(z)$ is the gamma function.

From the asymptotic properties of the Weber function[14], the general solutions of the Schrödinger equations (7a), (7b) and (7c) may take the following forms:

$$\chi_I(\xi) = A\, D_m(\xi) + B\, D_m(-\xi) \tag{13a}$$

$$\chi_{II}(\xi) = C\, D_m,(-\xi) \tag{13b}$$

$$\chi_{III}(\xi) = F\, D_m,(\xi) \quad , \tag{13c}$$

where A, B, C and F are the normalization constants in each region. Then the continuity of the logarithmic derivatives of the wave functions at both boundaries $\xi_L = \sqrt{2}a/a_H$ and $\xi_R = \sqrt{2}b/a_H$ of the quantum well provides the following equation for the energy eigenvalues:

$$D_m,(\xi_R)D'_m(\xi_R) - D'_m,(\xi_R)D_m(\xi_R)$$

$$= \frac{D'_m(\xi_L)D_m,(-\xi_L) + D'_m,(-\xi_L)D_m(\xi_L)}{D'_m(-\xi_L)D_m,(-\xi_L) + D'_m,(-\xi_L)D_m(-\xi_L)} \left[D'_m,(\xi_R)D_m(-\xi_R) + D_m,(\xi_R)D'_m(-\xi_R)\right] \quad , \tag{14}$$

where

$$D'_m(\xi) = \frac{d}{d\xi}D_m(\xi) \quad . \tag{15}$$

III. Results and Discussion

Making use of the recursion relations of the Weber function[14], the numerical solutions for m can be obtained from Eq. (14) if the values of V_0,

ξ_L and ξ_R are given. The numerical solutions of m are illustrated in Figs. (1) and (2) for different values of normalized potential height $V_0/\hbar\omega$ and well width W/a_H. We use the potential height $V_0 = 5\hbar\omega$ and the well width $W = a_H/\sqrt{2}$ in Fig. 1 and $V_0 = 10\hbar\omega$ and $W = \sqrt{2}a_H$ were used in Fig. 2. In these figures, the various energy levels are plotted against the position ξ_0 of the orbit center. In each graph the dotted line shows the boundaries of the quantum well on a normalized scale, and the quantum number m (y-axis) is related to the eigenenergy by $\epsilon = (m + 1/2)\hbar\omega$. These results clearly show two different types of energy states: (1) the states confined in the quantum well (the lowest level in Fig. 1 and the lowest two levels in Fig. 2) and (2) the extended states (the higher levels in Figs. 1 and 2).

For the confined states (1), most of the wavefunction is pushed into the quantum well because the eigenenergy is lower than the potential height. As the orbit center is shifted from the center of the potential well, the electron penetrates and spends increasingly more time inside the potential barrier and less time in the well, resulting thus in an increase of energy. If the orbit center is moved deep into the barrier and far away from the quantum well, the low-level electrons see essentially a magnetic harmonic well elevated by V_0. This means that the energy versus ξ_0 curve will flatten out at large values of ξ_0. Hence the usual bulk Landau levels take over except for a shift of V_0 in energy. Before the bulk Landau levels take over, we can see the crossing of the confined state and the extended state in the intermediate shift of orbit center ξ_0 in both Figs. 1 and 2. These two states are degenerate at the moment they cross each other. If the orbit center is shifted into the barrier, the quantum well would be elevated as

well as changed in shape by the presence of the parabolic magnetic potential. This means that the overall enhancement of the quantum well due to the magnetic potential should be parabolic as the orbit center ξ_0 is moving away from the quantum well. Thus the eigenenergies of the confined states in the quantum well increase parabolically as a function of the orbit center ξ_0. Clearly the crossings of the confined states and the extended states in Figs.1 and 2 exhibit parabolic behavior. The changes in shape of the quantum well neglecting the elevation have little effect on the crossings because the eigenenergies of the confined states are always limited by the barrier height V_0, which is small compared to the elevation due to the magnetic potential.

In the second case (2), the energy spacing between neighboring modes in the energy spectrum is about $\hbar\omega$, but each mode makes oscillations as the orbit center moves away from the center of the quantum well. In this case, the electron energies are higher than the potential height V_0 and the wavefunctions are located partly within the well and partly inside the barrier, but still confined by the magnetic potential well. The oscillatory behavior of the eigenmodes seems to be related to the oscillating property of the harmonic wavefunction. The harmonic wavefunction $[D_m(z)]$ has many nodes and peaks depending on the quantum number m, and the wavefunction may be classified as symmetric (even parity) or antisymmetric (odd parity) for the centered orbit (ξ_0=0). The oscillations of eigenenergy in each mode depend on the number of nodes on the wave function. Thus the number of oscillations increases one by one as we go up to the higher levels. We also observe that the oscillations of the eigenenergy are within the range of the

wavepacket size ($\Delta x = \sqrt{m+1/2}\ a_H$). The alternating downward and upward concavity in energy spectrum at the middle of the quantum well seems due to the symmetric or antisymmetric properties of the wavefunction. If the wavefunction is symmetric, the middle peak of the wavefunction is located at the center of the potential well for the centered orbit (ξ_0=0). Therefore the eigenenergy will increase if the orbit center is shifted slightly toward barrier, resulting in the downward concavity. On the other hand, we expect upward concavity for the antisymmetric wavefunction because its node is now located at the lowest spot of the combined potential well. If these arguments are correct, the wavefunction of the lowest mode should be symmetric and have no node, the second mode should be antisymmetric and have one node, and so on from Figs. 1 and 2. In conclusion, we can say that the energy levels with oscillating structures are direct images of the magnetic wave function itself in the restrcited geometry.

For the practical example of GaAs-Al_xGaAs_{1-x} with x = 0.3, we get V_0 = 0.25 eV. To match this potential height in fig.1 where $V_0 = 5\hbar\omega$, we need B = 29 T, which corresponds to a_H = 48 Å. If $V_0 = 10\hbar\omega$ like in Fig. 2, a magnetic field of B = 14 T is required. To observe these results at B = 10 T which has a magnetic length a_H = 81 Å, the potential height of Figs. 1 and 2 correspond to V_0 = 87 and 174 meV, respectively. Even if these results were calculated in a relatively strong magnetic field due to the computer limit, the general features could be observed in a practical samples given above.

Finally, the eigenenergies for an infinite potential well ($V_0 \rightarrow \infty$) can be calculated similarly with the proper boundary conditions ($\chi_{II} = \chi_{III} = 0$,

$\chi_I(\xi-\xi_R) = \chi_I(\xi-\xi_L) = 0$) and the results are presented in Fig. 3 with a well width $W = \sqrt{2}a_H$. In this case, since all the electronic motions are within the quantum well, we cannot see such extended states as for a finite potential height. As explained earlier, the parabolic behavior is almost the same except for higher energies than before due to the infinite well.

Acknowledgments

This research was supported by the Office of Naval Research and the Office of Air Force Office of Scientific Research (AFSC), United States Air Force, under Contract F49620-86-C-0009. The United States Government is authorized to reproduce and distribute reprints for governmental purposes, notwithstanding any copyright notation hereon.

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Figure Captions

1. Numerical solution for electron eigenenergy as a function of the orbit center ξ_0 with well width $W = a_H/\sqrt{2}$ and potential height $V_0 = 5\hbar\omega$.

2. Numerical solution for electron eigenenergy as a function of the orbit center ξ_0 with well width $W = \sqrt{2}/a_H$ and potential height $V_0 = 10\hbar\omega$.

3. Numerical solution for electron eigenenergy as a function of the orbit center ξ_0 with well width $W = \sqrt{2}/a_H$ and potential height $V_0 = \infty$.

Fig. 1

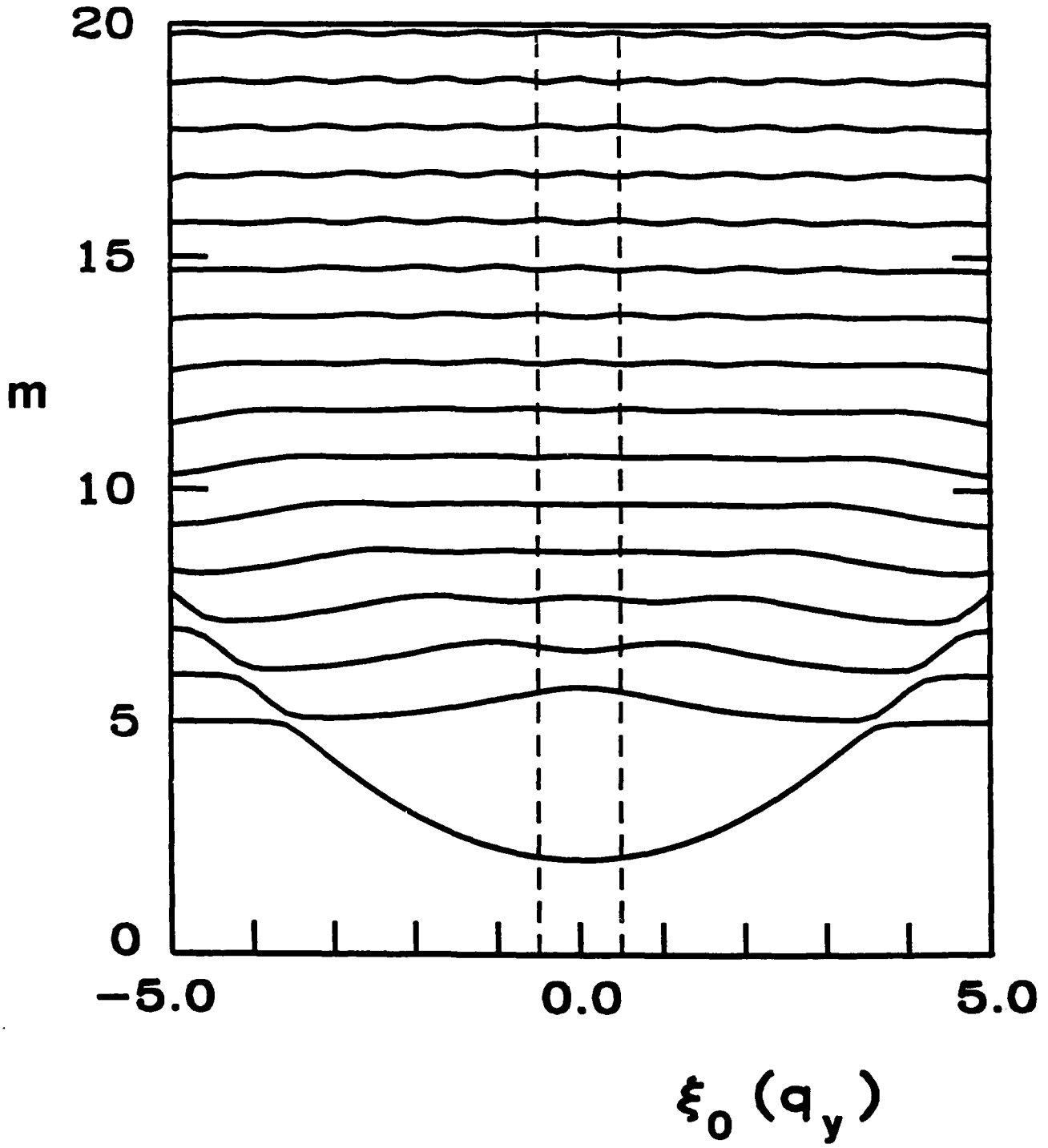


Fig. 2

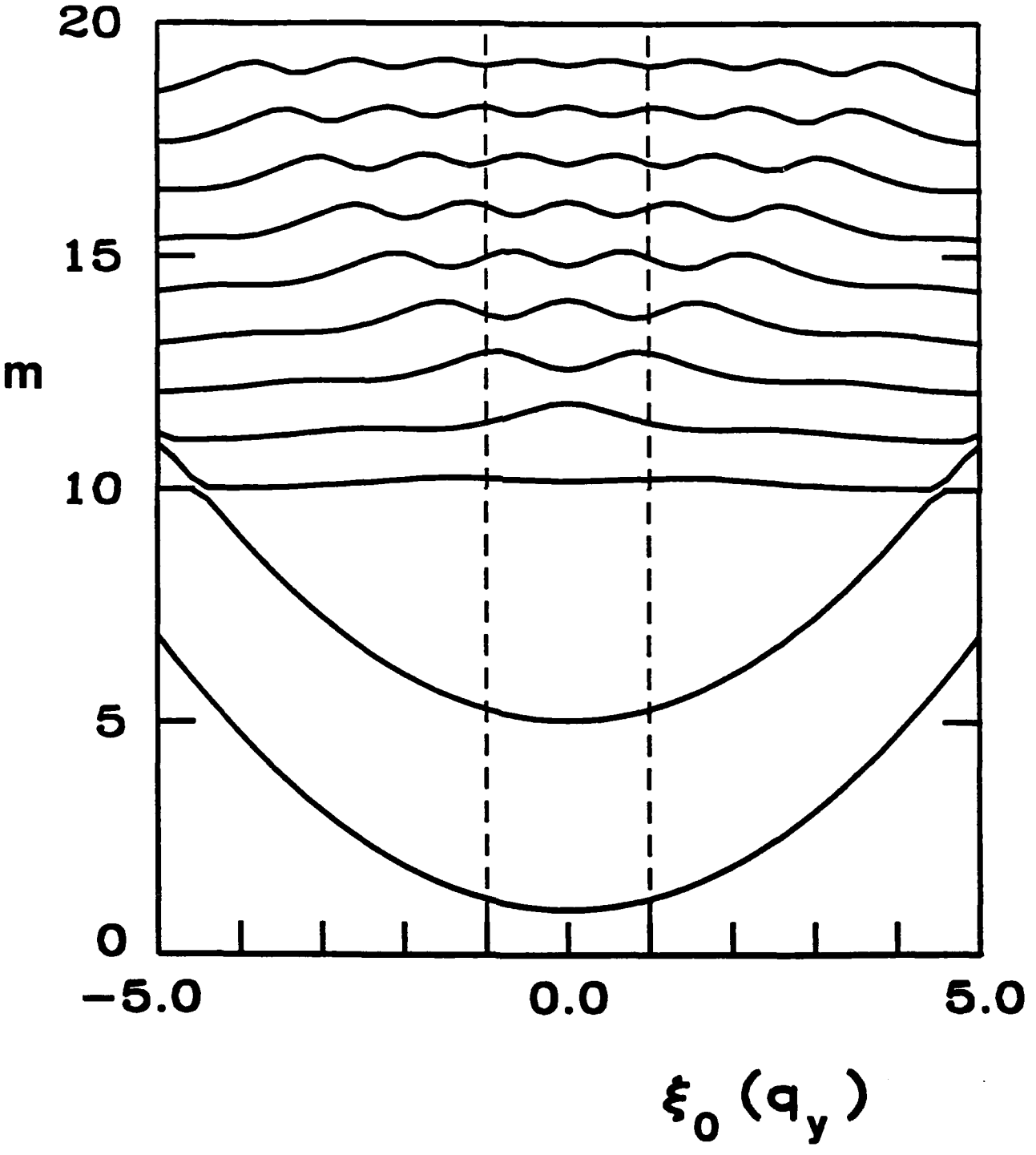
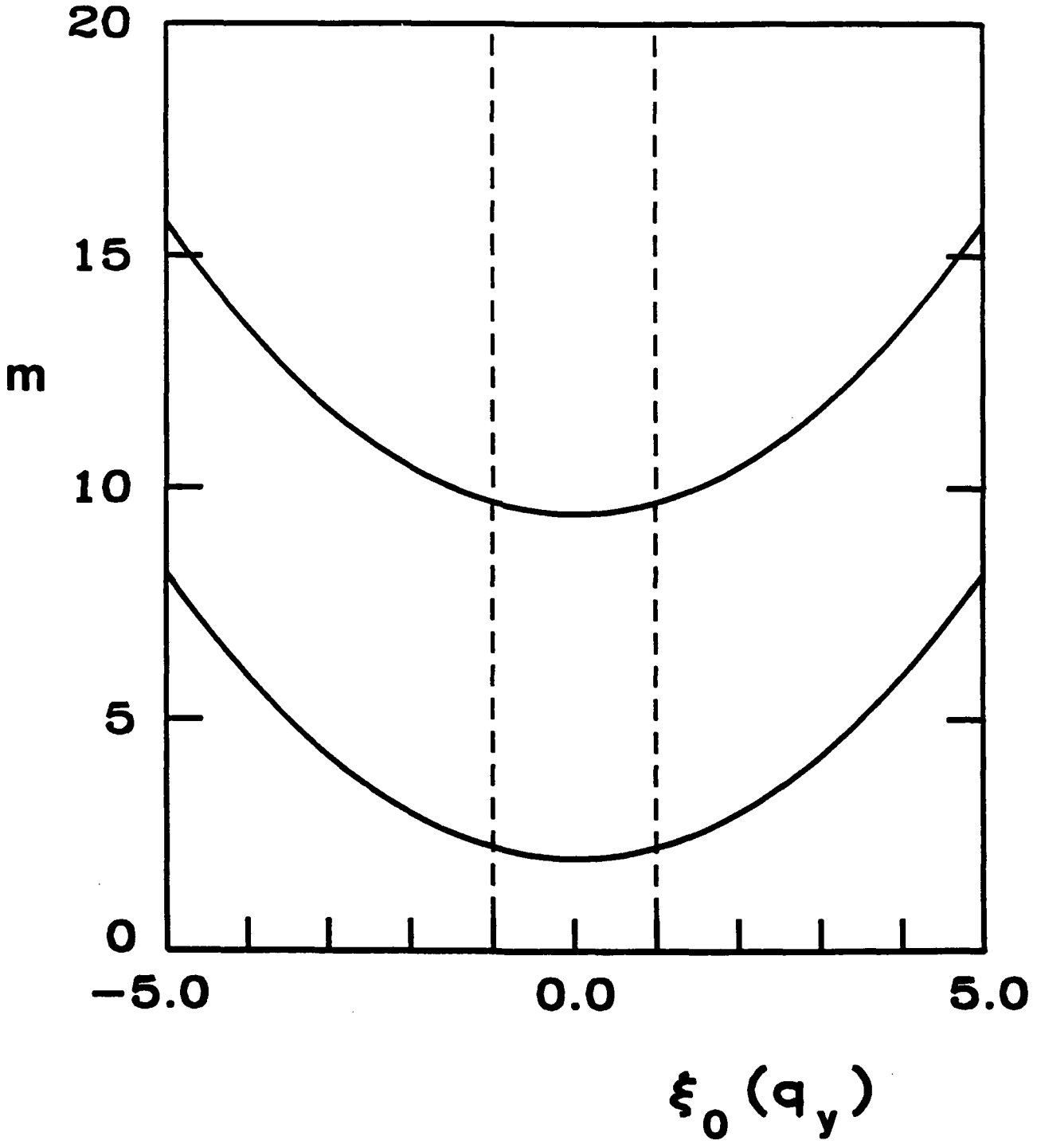


Fig. 3



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